Benzamide, 2,6-difluoro-3-methyl-N-(2,6-difluoro-3-methylbenz

Inchi: InChI=1S/C25H29F4NO2/c1-4-5-6-7-8-9-10-15-30(24(31)20-18(26)13-11-16(2)22(20)28)

InchiKey: ADXJWGFGPBUFDE-UHFFFAOYSA-N

Formula: C25H29F4NO2

SMILES: CCCCCCCCCN(C(=O)c1c(F)ccc(C)c1F)C(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 451.50

Physical Properties

Property code	Value	Unit	Source
gf	-599.64	kJ/mol	Joback Method
hf	-1097.16	kJ/mol	Joback Method
hfus	64.79	kJ/mol	Joback Method
hvap	92.03	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	6.893		Crippen Method
mcvol	335.790	ml/mol	McGowan Method
pc	1039.24	kPa	Joback Method
rinpol	2814.00		NIST Webbook
rinpol	2814.00		NIST Webbook
tb	971.90	K	Joback Method
tc	1189.91	K	Joback Method
tf	634.16	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.74	J/mol×K	971.90	Joback Method
cpg	1101.37	J/mol×K	1008.23	Joback Method
cpg	1114.83	J/mol×K	1044.57	Joback Method
cpg	1127.20	J/mol×K	1080.90	Joback Method
cpg	1138.52	J/mol×K	1117.24	Joback Method
cpg	1148.88	J/mol×K	1153.57	Joback Method
cpg	1158.33	J/mol×K	1189.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407762&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume